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## MEMORANDUM FOR PR (Contractor/In-House Publication)

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18 Apr 2000

SUBJECT: Authorization for Release of Technical Information, Control Number: **AFRL-PR-ED-AB-2000-075** Vij, V., Boatz, J.A., Tham, F., Vij, A., and Christe, K.O., "On the Lewis Acidity of LiF" (Abstract)

## 16<sup>th</sup> International Symposium of Fluorine Chemistry (Durham, UK, 23 Jul 00) (Submission Deadline: 18 Apr 2000)

(Statement A)

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## ON THE LEWIS ACIDITY OF LIF

V. Vij, , J. A. Boatz, F. Tham, A. Vij and K. O. Christe\*

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Based on the recently developed pF Lewis acidity scale, free gaseous LiF is a surprisingly strong Lewis acid, comparable to SiF<sub>4</sub>. It was therefore of interest to study whether a strong Lewis base, such as CsF, could transfer a fluoride ion to LiF with formation of a LiF<sub>2</sub> anion. Theoretical calculations were carried out for LiF<sub>2</sub> and show that free gaseous LiF<sub>2</sub> is a linear, vibrationally stable species. Furthermore, the phase-diagram of the LiF/CsF system shows a eutectic at a 1:1 mole ratio that gives a distinct X-ray powder diffraction pattern. We have prepared this eutectic by fusion of a 1:1 mixture of LiF and CsF in a platinum crucible. Single crystals were obtained by slow cooling of the melt in a dry nitrogen stream. The resulting product was characterized by vibrational spectroscopy, and its crystal structure was determined. It is shown that CsLiF<sub>2</sub> does not contain isolated LiF<sub>2</sub> anions, but exhibits an interesting three-dimensional network of alternating tetra-coordinated LiF<sub>4</sub> and octa-coordinated CsF<sub>8</sub> units.

<sup>1.</sup> K. O. Christe, D. A. Dixon, D. McLemore, W. W. Wilson, J. A. Sheehy and J. A. Boatz, J. Fluorine Chem., 2000, 101,151.

<sup>2.</sup> D. L. Deadmore and J. S. Machin, J. Phys. Chem., 1960, 64, 824.